Quantum Annealing: The Quantum Solution to Optimization and Empirical Comparisons with Classical Methods

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Abstract

Quantum Annealing (QA) is a promising approach to tackle complex optimization problems by leveraging quantum mechanical phenomena such as superposition, entanglement, and quantum tunneling. In this paper, we delve into the mathematical core of QA, exploring its underlying quantum mechanical operations and clarifying its effectiveness in optimization tasks. Furthermore, we present our own simulations and empirical analysis, comparing the performance of QA and classical annealing techniques, particularly Simulated Annealing (SA), on linear systems of equations and the knapsack problem. Based on analysis, we highlight the advantages and limitations of QA, briefly touch upon its industry applications, and expand upon the potential of QA in revolutionizing optimization strategies while considering the future trajectory of quantum computing technologies.

Contribution Statement

As the authors of this study, our primary objective was to create a valuable resource for beginners in quantum computing, early career academic researchers, and various industry professionals. We aim to provide a clear, interpretable, and comprehensive overview of quantum annealing, and also showcase some practical scenarios. We believe that providing such insights can significantly benefit various professionals by enhancing their understanding of quantum computing's potential applications and implications that could range from business to investment decisions.

1 Introduction

Combinatorial optimization problems are central to many real-world applications, ranging from logistics, finance, and beyond. These problems involve the arrangement and selection of the optimal element from a finite set of elements to optimize a certain objective such as maximizing efficiency, or achieving the best possible outcome. Classical algorithms often struggle to find optimal solutions within a reasonable time frame for complex problem instances. Recognizing the potential of quantum computing to tackle such challenges, our motivation in this paper is to explore the intersection of these problems with quantum mechanics' properties.

1.1 Background

QA is a heuristic quantum optimization algorithm tailored to solve combinatorial optimization problems specifically, unlike a universal gate model quantum computer; some examples are finding the ground state of traveling salesman or a spin glass problem. Performed by the quantum annealer hardware, QA involves evolving a collection of qubits, the quantum system, from initial state to a final state that represents the solution to the problem. The concept of quantum annealing metaphorically gets its name from the physical process of annealing in metallurgy, where a metal is gradually cooled to achieve a desired structure. In QA, analogously, the system tries to arrive at the minimum energy state that corresponds to the optimal solution of the problem Hamiltonian by decreasing the energy of the system infinitesimally slow.

The process of quantum annealing, as developed by Kadowaki and Nishimori (1998) (1), starts with qubits in superposition to represent all possible answers. As the annealing goes on, biases and couplings between qubits are adjusted by the annealer. Biases refer to external magnetic fields applied to individual qubits, effectively setting the preference for each qubit's state. Couplings are the interactions between pairs of qubits, determining how the state of one qubit influences another, which directly shapes the multi-qubit landscape of potential solutions (2). These modifications tilt the energy landscape, making certain solution states more energetically favourable than others. One can understand this better with an analogy of a mountain range with valleys and peaks that correlate with different solution states. The optimal solution can be thought of as the bottom of the valley with lowest altitude in the whole mountain range. During this evolution of the system, qubits become entangled with each other as a natural consequence of the quantum dynamics governed by the Hamiltonian of the system, which we will dive more deeply in the following sections of the paper; this entanglement of qubits allows for the quantum system to represent complex multi-qubit interactions that define the problem and its constraints.

Achieved by superposition and quantum tunneling—phenomena central to attaining a quantum advantage—the system's exploration of the energy landscape is governed by the time-dependent Schrödinger equation, which describes how quantum states evolve in response to a dynamically changing Hamiltonian. This evolution is guided by the adiabatic theorem (3), ensuring the system to not lose the problem configuration with time. As the problem reaches minimum energy, each qubit settles into a classical state that represent the best configuration found in this quantum exploration.

1.2 Prior and Current Work

The field of quantum annealing and its applications in optimization have roots in early computational methods. The equation-of-state calculations proposed by Metropolis et al. (5) laid the foundation for numerical computations. However, it is essential to note that this field is still in its nascent stages.

The seminal work by Kadowaki and Nishimori (1) introduced the algorithm of quantum annealing, sparking significant interest in the field. Subsequent influential works by Brooke et al. (6) and Farhi et al. (7), further explored the potential of quantum annealing in solving complex optimization problems.

Another significant advancement was proposed by Farhi et al. (3), outlining a procedure for adiabatic quantum optimization. This work paved the way for further research and development in quantum optimization techniques.

Nowadays, in addition to academic research, quantum annealing has gained traction in industry applications, particularly through D-Wave Systems (8), which provides a vertical stack of technologies from hardware to cloud services specifically on quantum annealing.

1.3 Simulated Annealing

Simulated Annealing (SA), on the other hand, is the classical counterpart of QA. It is a widely-used classical optimization algorithm, which is used to find the minimum of a function and is applicable in many industries. This technique was first articulated by Kirkpatrick, Gelatt, and Vecchi in 1983 (4).

The main working principle behind SA is the adjustment of a "temperature" parameter, which at first makes it possible for the algorithm to accept both better and worse solutions with a high probability, allowing for a thorough investigation of the solution space. The algorithm becomes less tolerant to sub optimal solutions as the temperature decreases and becomes more conservative, increasing its focus on regions of the solution space that offer lower energy states. This regulated cooling schedule improves the algorithm's ability to locate a global minimum by gradually reducing the likelihood that it will become stuck in a local minimum.

A key distinction between Simulated Annealing (SA) and Quantum Annealing (QA) is that SA, being a classical algorithm, cannot utilize quantum tunneling, which is a phenomenon exclusive to quantum systems. SA operates on classical bits and relies on probabilistic transitions over energy barriers to explore the solution space. In contrast, QA leverages quantum bits (qubits) and can exploit quantum tunneling, where the system can transition directly through energy barriers to another state (11). This capability allows QA to potentially find optimal or near-optimal solutions more efficiently by avoiding being trapped in local minima, a common challenge in classical optimization algorithms.

Due to its simplicity and robustness and practical availability for deployment on classical hardware, SA is suitable for a variety of complex optimization problems, providing superior solutions than many other methods.

2 Theoretical Foundations

2.1 Mathematical Core

In quantum annealing, the behavior of the system is governed by the system Hamiltonian, which dictates how it evolves over time towards the lowest energy state (3). The Hamiltonian comprises two main components: the initial Hamiltonian, H_{init}, which represents a simple ground state and the problem Hamiltonian, H_{prob}, which is the Hamiltonian whose ground state represents the optimal solution to out problem. combined as follows:

$$H(s) = A(s)H_{\text{init}} + B(s)H_{\text{prob}}$$

where s is a parameter that drives the time-dependent scaling functions of A(s) and B(s). Those functions orchestrate the evolution of the system's Hamiltonian, steering it from H_{init} as decreases A(s) to H_{prob} as B(s) increases which handle the evolution of our system Hamiltonian.

2.1.1 Initial Hamiltonian H_{init}

The initial Hamiltonian sets the quantum system in a superposition of all possible states, essential for quantum parallelism. It is given by:

$$H_{\text{init}} = -A(s)\sum_i \sigma_i^x$$

where σ_i^x is the Pauli-X matrix, acting as a quantum bit-flip operator:

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

which toggles qubits between their $|0\rangle$ and $|1\rangle$ states, creating superpositions when applied to any quantum state (2).

2.1.2 Problem Hamiltonian H_{prob}

This Hamiltonian encodes the specific optimization problem and shapes the energy landscape:

$$H_{\text{prob}} = B(s)\left(\sum_i h_i\sigma_i^z + \sum_{i<j} J_{ij}\sigma_i^z\sigma_j^z\right)$$

Here, σ_i^z and σ_j^z are the Pauli-Z matrices for qubits i and j, respectively and are critical for encoding the specific constraints and objectives of the problem.

The Pauli-Z matrix, σ^z, defined as:

$$\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

operates on the computational basis states by assigning them eigenvalues of +1 and -1, corresponding to the classical binary states 0 and 1, respectively. This binary distinction is fundamental in mapping classical optimization problems onto quantum systems (2).

The coefficients h_i and J_{ij} play distinct roles:

- The h_i coefficients represent external magnetic fields affecting individual qubits, effectively biasing each qubit towards one of its two possible states (0 or 1). (3).

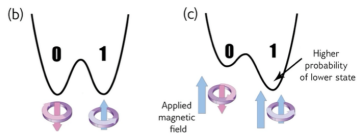


Figure 1: Visual representation of the magnetic fields' effect on the energy landscape of the system Hamiltonian (20).

- The J_{ij} coefficients represent the interaction strengths between pairs of qubits. These terms are crucial for encoding the relationships and dependencies between variables in the original optimization problem (3).

These coefficients h_i and J_{ij} are predetermined values specifically tailored to encode the constraints of the problem. The accurate configuration of these parameters are important for the quantum annealer to effectively find the optimal solution.

2.1.3 Annealing Schedule

The functions $A(s)$ and $B(s)$ define the annealing schedule, controlling the evolution of the Hamiltonian from H_{init} to H_{prob} (12). They are typically chosen to ensure a smooth transition that satisfies the adiabatic theorem, crucial for keeping the system in its lowest energy state. $A(s)$ generally starts high and decreases, while $B(s)$ starts low and increases as the annealing process progresses.

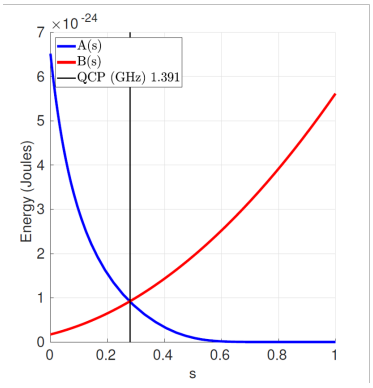


Figure 2: The interplay between the annealing functions $A(s)$ and $B(s)$ as the annealing schedule progresses (20).

As the annealing process unfolds (Figure 2), A(s) diminishes, reducing the influence of the initial Hamiltonian and the superposition state, while B(s) grows, increasing the problem Hamiltonian's influence and steering the system towards a state that represents the problem's solution. The interplay between A(s) and B(s) through the annealing schedule controls the quantum system's evolution to find the lowest energy state and the solution to the optimization problem (12) (8).

2.2 Quantum Tunneling: The Heart of Quantum Annealing

Quantum annealing leverages quantum tunneling to efficiently solve optimization problems with complex energy landscapes. This process allows quantum annealers to pass directly through energy barriers rather than climbing over them, which is a significant advantage over classical algorithms. This feature is crucial in reaching global minima more effectively and is highlighted in the study by Johnson et al.(13), who demonstrate quantum annealing's superior performance in certain optimization scenarios.

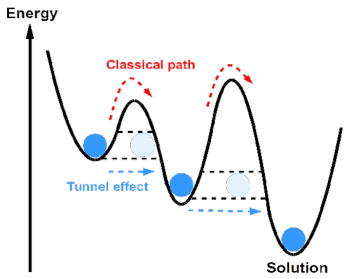


Figure 3: Conceptual illustration of quantum tunneling (21)

Hybrid quantum-classical approaches that combine quantum annealing with classical algorithms offer a promising solution to exploit the strengths of both technologies. These hybrid systems utilize quantum tunneling for navigating complex parts of the solution space, while classical algorithms refine these solutions. A notable discussion on this can be found in Farhi et al.'s work (15).

The implications of quantum tunneling for industries like finance, logistics, and materials science are profound, with potential for improvements in processing times. This is explored in detail by Venturelli and Kondratyev (16).

For readers interested in delving deeper into the mathematical background of quantum tunneling, a thorough understanding of quantum mechanics is needed. The review by Albash and Lidar (14) provides a comprehensive mathematical treatment of these principles.

2.3 Adiabatic Theorem: Ensuring Ground State Evolution

The foundational piece that holds the algorithm together is the Adiabatic Theorem for quantum states. In this section, we shall describe it's mathematical core. Before diving into that, one can start building their intuition of the concept by observing the following real-world analogy. In the context of a pendulum motion, if the control arm of the pendulum is shortened slowly enough, the motion of the pendulum won't get affected. The same applies for quantum states, which we shall detail in the next paragraphs.

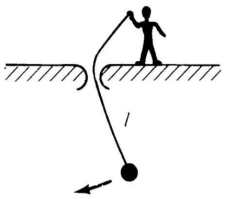


Figure 4: Analogical example of the adiabatic theorem (22)

In his 1958 paper, Kato provided important insight into the evolution of quantum systems under slow varying Hamiltonians by proving that the quantum system remains in its instantaneous eigenstate when the Hamiltonian governing the system changes slowly enough and has a nonzero gap with the other states. (17). This is particularly crucial for quantum annealing processes to work smoothly because, as the system finishes evolving from H_{init} to H_{prob}, the adiabatic theorem ensures that the system will continue to remain in the ground state of the evolving Hamiltonian, which eventually corresponds to the ground state of H_{prob}, mapping to our solution space.

Before diving deeper into Kato's dynamics, we shall layout the general adiabatic theorem for the quantum states by refering to the Applications of Quantum Mechanics course at TU Delft (18). Our system starts with the time-dependent Schrödinger equation which represents our system.

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = H(t)|\Psi(t)\rangle$$

To solve the this time-dependent problem, let's define E(s) to be the eigenvalues of our Hamiltonian at time s and $\psi_n(t)$ to be the eigenstates of the corresponding eigenvalues.

$$H(t)\psi_n(t) = E_n(t)\psi_n(t)$$

Now, expressing our quantum state as a linear combination of it's eigenstates as the eigenstates form a complete orthonormal set

$$\Psi(t) = \sum_n c_n(t)\psi_n(t)e^{i\theta_n(t)}$$

We can apply the time-dependent Schrödinger equation to the representation of our system with the linear combination of it's eigenstates, this will allow us to analyze our system's coefficients' $\dot{c}_n(t)$ evolution over time. This is particularly useful as the absolute square (amplitude) $\dot{c}_n(t)$ provides the possibility of finding the system at $\psi_n(t)$ upon measurement.

$$i\hbar\sum_n \left[\dot{c}_n\psi_n + c_n\dot{\psi}_n + c_n\psi_n i\dot{\theta}_n\right] e^{i\theta_n(t)} = \sum_n c_n(t)H(t)\psi_n(t)e^{i\theta_n(t)}$$

which simplifies to

$$\sum_n \dot{c}_n\psi_n e^{i\theta_n} = -\sum_n c_n\dot{\psi}_n e^{i\theta_n}$$

Now we are going to project this expression on to the ψ_m eigenstate. This is particularly helpful as we want to observe how $\dot{c}_m$ is affected by the evolution of the Hamiltonian. This way, we can

determine the necessary conditions under which the change in $\dot{c}_m$ are negligible. If we can manage to find those conditions, this will lead us to the adiabatic theorem, which ensures that system will maintain its projection onto the same or corresponding eigenspace over time.

$$\dot{c}_m = -\sum_n c_n \langle \psi_m | \dot{\psi}_n \rangle e^{i(\theta_n - \theta_m)}$$

Now we project the derivative of the initial time-dependent Schrödinger equation on to ψ_m to find $\langle \psi_m | \dot{\psi}_n \rangle$

$$\langle \psi_m | \dot{H} | \psi_n \rangle + E_m \langle \psi_m | \dot{\psi}_n \rangle = \dot{E}_n \delta_{nm} + E_n \langle \psi_m | \dot{\psi}_n \rangle$$

which, for n $\neq$ m

$$\langle \psi_m | \dot{\psi}_n \rangle = \frac{\langle \psi_m | \dot{H} | \psi_n \rangle}{(E_n - E_m)}$$

When the evolution of the system is slow and gradual, H is small and other coefficients' contributions are negligibly small if n $\neq$ m. This provides us with the following result

$$\dot{c}_m = -c_m \langle \psi_m | \dot{\psi}_m \rangle.$$

The above result shows the changes in the $\dot{c}_m$ coefficient are governed primarily by the direct time evolution of the state itself and not by transitions between different states due to off-diagonal Hamiltonian contributions. This shows us that the probability of projecting on to ψ_m is primarily influenced by the internal dynamics of itself.

To connect our findings to the Kato's quantum adiabatic theorem proof, we need to notice that each eigenstate evolving independently from others imply that the system's evolution can be explained as a unitary transformation since each transformation acts on a particular eigenstate and doesn't cause any mix or leakage.

Knowing that our system's evolution doesn't mix the eigenstates, we can imply that the evolution operation preserves the orthogonality and normalization of the state vectors, which is another characteristics of an Unitary operation.

Now let W(s) be represent the unitary evolution of our system Hamiltonian to a lower energy system

Theorem 17.3 (Kato dynamics): Let $W(s)$ solve the differential equation:

$$\frac{dW}{ds} = iA(s)W(s), \quad 0 \leq s \leq 1; \quad W(0) = I,$$

where

$$iA(s) = [P'(s), P(s)].$$

Then $W(s)$ is unitary and obeys:

$$W(s)P(0)W(s)^{-1} = P(s).$$

The proof demonstrates that if the derivative of the evolution operator $W(s)$ adheres to the commutator $iA(s)$, then the system's initial projection onto an eigenspace at $s = 0$ is preserved throughout the evolution up to $s = s$. This means that the eigenspace in which the system begins remains consistent after the system evolves, thereby maintaining the same eigenspace projection throughout the evolution process, which proves how we are able to reach to the correct problem configuration at H_{prob}.

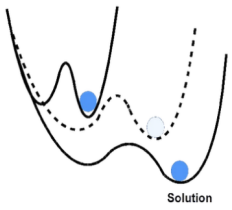


Figure 5: Visual description of the evolution of the system to a lower energy state

3 Main Results and Comparative Analysis

In our research, we conducted two different simulations to examine the performance and efficiency of Quantum Annealing (QA) compared to classical methods.

3.1 Solving Linear Systems

In this segment of our study, we evaluated the performance of Quantum Annealing (QA) and Simulated Annealing (SA) for solving linear systems represented by the equation $Ax = b$. The matrices A and vectors b were generated randomly for each of the 10 iterations to simulate a variety of scenarios. This approach ensures that the findings are more robust.

Each linear system was transformed into a Quadratic Unconstrained Binary Optimization (QUBO) problem to facilitate processing on a quantum annealer. The transformation into QUBO format is crucial as it aligns the problem with the operational capabilities of quantum hardware, particularly the D-Wave systems used in our experiments. The matrices and vectors involved in the QUBO formulations represented constraints and objectives derived from the original linear systems. The code for this simulation can be found in the Appendix.

3.1.1 Experimental Setup and Results

- **Matrix and Vector Generation:** The matrix A and vector b in each iteration were created using a pseudo-random number generator, ensuring a wide range of test conditions. Each matrix was square, with dimensions progressively increasing from 4×4 to 16×16 to incrementally challenge the annealers with increasing complexity.
- **2-Norm of Residuals:** We measured the effectiveness of each solution by calculating the 2-norm of the residual $r = Ax - b$, where x is the solution provided by the annealers. The residual norms provide a quantitative measure of the accuracy of the solutions.
- **Number of Bits:** The number of bits used to represent each variable in the QUBO problem was varied from 2 to 10. This variation tests the impact of solution granularity on the accuracy of both QA and SA.
- **Computation Time:** Time efficiency was another critical aspect of our evaluation, with total computation time recorded for each iteration, providing insights into the scalability and practicality of using quantum resources for linear system solutions.

In addition to QA and SA, the NumPy solver, utilizing the least squares method, was also employed and serving as the benchmark.

3.1.2 Analysis and Implications

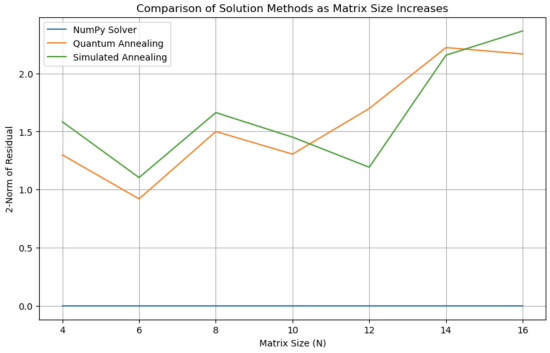


Figure 6: Performance vs. Matrix Size (N) of QA and SA. Number of bits used is fixed to 4 (num_bits = 4).

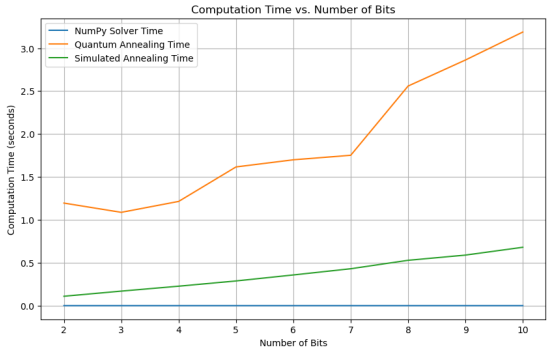
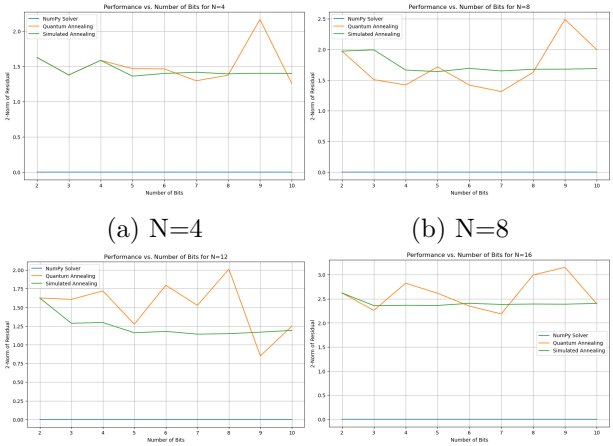


Figure 7: Computation Time (s) vs. Number of Bits of QA and SA. Matrix size is fixed to N=4

The experimental data yielded several key insights into the performance dynamics of QA and SA under varying conditions.

Figure 6 demonstrates that as matrix size increases from $N = 4$ to $N = 10$, QA performs slightly better than SA. The similar trajectories of QA and SA within this interval suggest comparable behaviors under these conditions. After $N = 10$, SA performs with higher accuracy until



(a) N=4 (b) N=8

(c) N=12 (d) N = 16

Figure 8: Performance vs. Number of Bits plots of QA and SA for four different scenarios. Matrix size is fixed per plot and 2-norm solution is examined as number of bits increases.

$N = 14$, supporting the claim that SA often provides more accurate results as the complexity of the problem increases. Contrary to this claim, after $N = 14$, QA deviates and provides superior results. Thus, after $N = 10$, the most high-level analysis would be that they perform quite comparably as the problem complexity increases. The slight superiority of QA until $N = 10$ and the comparable performance thereafter highlight the potential in Quantum Annealing for solving complex optimization problems.

The computation time for QA increased with the number of bits (Figure 7), which was anticipated given the quantum computation processes involved (3). SA performed consistently faster, aligning with previous findings that classical algorithms can often execute more quickly when quantum advantages do not strongly manifest (4). This observation is supported by the nature of the quantum annealing process, which, while potent, involves a more complex setup and execution compared to classical simulated annealing techniques, as discussed in (14).

While one might expect QA and SA to show improved results with the increase in bits due to enhanced granularity in solution representation, the plots in Figure 8 reveal that this is not necessarily the case. For all matrix sizes, the performance of QA and SA does not exhibit a consistent improvement as the number of bits increases. This observation might be attributed to the inherent simplicity of the linear system being solved, which do not fully exploit the capabilities of more complex solution representations.

3.2 Methodological Limitations

The linear system in this study, while varied in size, was inherently linear and relatively straightforward; nonlinear problems, often more complex and challenging, may provide more insightful results.

Due to the constraints on the availability of quantum computing resources on D-Wave quantum system, our experiments were limited to 10 iterations per scenario. This small sample size might not adequately represent the statistical variability and could affect the reliability and accuracy of the findings. Expanding the number of iterations in future studies would help achieve a more robust statistical analysis and validate the consistency of the observed results.

3.3 Knapsack Problem

We deployed both the QA and classical approaches to further observe the results over the infamous Knapsack problem. The reason we choose the Knapsack problem is because it's an NP-Complete problem that has wide applications in different branches of industry.

As for QA solution, we utilized D-Wave System's Hybrid Constrained Quadratic Model (CQM) solver, and for the classical counterpart, we utilized a naive knapsack dynamic programming approach O(nW). The following are the times that it took both algorithms to arrive at the optimal solution on growing sizes of weights.

As demonstrated in Table 1, the performance of classical and QA (hybrid for this case) models varies significantly across different problem sizes. For smaller problems, classical approach was significantly faster.

Problem Size	Time Taken (Classical)	Time Taken (QA)
2	$6.89e^{-5}$ s	7.11 s
7	0.00217 s	7.06 s
68	0.636 s	7.30 s
653	648.58 s	7.53 s
3338	N/A	7.78 s

Table 1: Time Taken for Classical and Quantum Annealing (QA)

However, as the problem size increases, the time taken by the classical model escalates drastically, resulting in N/A due to the classical model's inability to complete the task within a reasonable timeframe.

In contrast, QA maintains a relatively constant time across all problem sizes, including large ones. This indicates a significant advantage of QA: its scalability and robustness in handling complex combinatorial optimization problems without a substantial increase in computational time. The fact that time taken remained constant might be due to time taken in initializing, setting up, and executing the quantum model rather than the complexity of the problem.

4 Discussion

The findings of Linear System formulation elucidate the trade-offs between computational speed and accuracy within Quantum and Simulated Annealing. While QA achieved comparable, slightly better accuracy when problem got more complex, its slower computation times highlight the current practical limitations of quantum technologies.

These results of are not conclusive and indicate the need for further experimentation. Future studies for solving linear systems of equations should consider more complex linear and possibly non-linear systems where the increased granularity of solution representation might play a more crucial role. Additionally, expanding the scale of experiments to include a broader range of matrix sizes and conditions could provide deeper insights into the capabilities and limitations of quantum and simulated annealing in this context.

The findings on the Knapsack problem are particularly promising for the future of quantum computing in fields that require solutions to large-scale, complex problems. The ability of QA to work well in hybrid with classical algorithms further sheds light on how well these collaborations work in many scenarios.

Future studies should aim to further investigate the scaling properties of QA compared to classical approaches, particularly focusing on the cost-benefit analysis of quantum computing for medium-sized problems where classical solutions are still feasible but potentially less efficient.

5 Conclusion

In this study, we have systematically explored the mathematical core of the quantum annealing method for optimization problems, and explained the quantum properties that enable this algorithm. In addition, we have conducted real world cases to explore the results for possible implications.

Although it is possible to witness quantum speedups in certain case studies, one can criticize them such cases for not being practically scalable. Main barrier of their scalability, mainly in Quantum Annealer, is the amount of fine-tuning it requires to execute a query as the biases and couplings of the QPU (8) needs to be predetermined since it's static unlike the weights of traditional machine learning models. On top of that, as our results show, competing with the numerical optimization of the classical solvers (NumPy) is a challenging task for the current quantum algorithms.

However, a promising finding lies at the overlap of quantum and classical algorithms (hybrid). As the hybrid solutions use classical resources to find problems' hard cores and use the quantum

resources to execute them as small pieces (19), makes them a viable option to consider for input sizes above certain range because of the overhead this orchestration requires at each execution.

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[21] Source: Quantum World Association

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